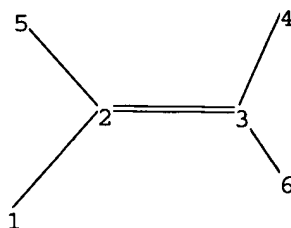
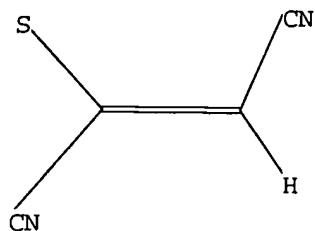


10519823 6/6/06

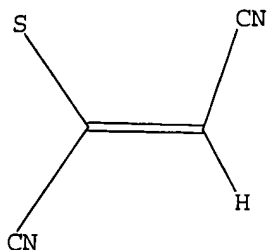


chain nodes :
1 2 3 4 5 6
chain bonds :
1-2 2-3 2-5 3-4 3-6
exact/norm bonds :
2-5
exact bonds :
1-2 2-3 3-4 3-6

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 13:11:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 55 TO ITERATE

100.0% PROCESSED 55 ITERATIONS
SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 656 TO 1544
PROJECTED ANSWERS: 1 TO 80

10519823 6/6/06

L2 1 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 13:11:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1007 TO ITERATE

100.0% PROCESSED 1007 ITERATIONS 11 ANSWERS
SEARCH TIME: 00.00.01

L3 11 SEA SSS FUL L1

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	167.15

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=> s l3
L4 5 L3

=> d ibib abs hitstr tot

10519823 6/6/06

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:17419 CAPLUS

DOCUMENT NUMBER: 140:77143

TITLE: Process for the preparation of phenylpyrazoles and dicyanoalkylthioethene intermediates.

INVENTOR(S): Ancel, Jean-Erick; Vidal, Joselle

PATENT ASSIGNEE(S): Bayer CropScience SA, Fr.

SOURCE: Eur. Pat. Appl., 7 pp.

CODEN: EPXOXW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1378506	A1	20040107	EP 2002-356131	20020705
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CA 2490987	AA	20040115	CA 2003-2490987	20030630
WO 2004005245	A1	20040115	WO 2003-EP8212	20030630
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RV: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TH, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003250177	A1	20040123	AU 2003-250177	20030630
BR 2003012469	A	20050503	BR 2003-12469	20030630
CN 1665781	A	20050907	CN 2003-815996	20030630
JP 2005532384	T2	20051027	JP 2004-518774	20030630
US 2006052614	A1	20060309	US 2005-519823	20050713
PRIORITY APPLN. INFO.: EP 2002-356131 A 20020705				
WO 2003-EP8212 W 20030630				

OTHER SOURCE(S): CASREACT 140:77143; MARPAT 140:77143

AB RS(NC)C:CHCN (R = CF₃, alkyl) were prepared by reaction of NCC.tpbond.CCN with RSM (R as above; M = alkali metal, alkaline earth metal, Ag). Thus, CF₃SAg in acetone at -78° was added to dicyanoacetylene and H₂O in acetone; the resulting mixture was shaken for 12 h to give 39% 1,2-dicyano-1-trifluoromethylthioethene. This and 2,6-dichloro-4-trifluoromethylphenylhydrazine were stirred in THF for 24 h to give 12% 1-(2,6-dichloro-4-trifluoromethylphenylhydrazino)-1,2-dicyano-2-trifluoromethylthioethane. This was heated with CuCl₂ in PhCl at 100° for 4 h to give 65% 5-amino-3-cyano-1-(2,6-dichloro-4-trifluoromethylphenyl)-4-trifluoromethylthiopyrazole after recrystn.

IT 642097-20-9P

RL: IMP (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (process for the preparation of phenylpyrazoles and dicyanoalkylthioethene intermediates)

RN 642097-20-9 CAPLUS

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:662869 CAPLUS

DOCUMENT NUMBER: 139:323278

TITLE: A Forbidden Rearrangement

AUTHOR(S): Leivers, Martin; Tam, Iris; Groves, Kevin; Leung, David; Xie, Yuli; Breslow, Ronald

CORPORATE SOURCE: Department of Chemistry, Columbia University, New York, NY, 10027, USA

SOURCE: Organic Letters (2003), 5(19), 3407-3409

CODEN: ORLEP7; ISSN: 1523-7060

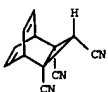
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

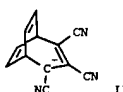
LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:323278

GI



I



II

AB The barrelene derivative I fragments to afford benzene and trappable 1,2,3-tricyanocyclopropene, whereas its anion fragments more easily to liberate benzene and the 1,2,3-tricyanocyclopropenyl anion, which is not trappable or stable in solution. However, the major thermal product from the barrelene anion is a rearranged allyl anion II that is formed by disrotatory cleavage of the cyclopropyl ring, a formally Woodward-Hoffmann-forbidden process. Several proposals are offered to rationalize this forbidden rearrangement.

IT 612484-26-1P

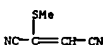
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(cyclopropanation; preparation of tricyanobicyclo[3.2.2]nonatriene

derivs. via forbidden rearrangement of tricyanocyclopropabarrelene)

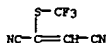
RN 612484-26-1 CAPLUS

CN 2-Butenedinitrile, 2-(methylthio)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 2-Butenedinitrile, 2-[(trifluoromethyl)thio]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1979:550400 CAPLUS

DOCUMENT NUMBER: 91:150400

TITLE: Phthalocyanines and related compounds XVI. Synthesis and electronic absorption spectra of amino-, alkoxy-, and alkylthio-substituted porphyrans

AUTHOR(S): Kopranev, V. N.; Goncharova, L. S.; Luk'yanets, E. A.

CORPORATE SOURCE: Nauchno-Issled. Inst. Org. Poluprod. Krasitelei, Moscow, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1979), 15(5), 1076-82

CODEN: ZORXAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB During the reactions of mono- and dichloromaleonitriles or fumaronitriles with NaOBu-tert and Na tert-thioamylate and tert-butylamine, mono- and disubstituted nitriles were obtained which were used to prepare tetra- and octasubstituted porphyrans Mg complexes. The substituent in the macrocycle of the porphyrans has a large effect on its electronic absorption spectrum.

IT 71200-71-0P

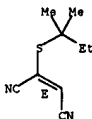
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and template reaction of)

RN 71200-71-0 CAPLUS

CN 2-Butenedinitrile, 2-[(1,1-dimethylpropyl)thio]-, (E)- (9CI) (CA INDEX NAME)

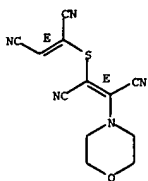
Double bond geometry as shown.



10519823 6/6/06

L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1970:466519 CAPLUS
 DOCUMENT NUMBER: 73:66519
 TITLE: Aminolysis of tetracyano-1,4-dithiin with secondary amines
 AUTHOR(S): Fickentscher, Kurt; Fehlhaber, Hans W.
 CORPORATE SOURCE: Pharm. Org.-Chem. Inst., Univ. Bonn, Bonn, Fed. Rep. Ger.
 SOURCE: Justus Liebig's Annalen der Chemie (1970), 736, 176-80
 CODEN: JLABCF; ISSN: 0075-4617
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 73:66519
 AB Reaction of 1 mole tetracyano-1,4-dithiin (I) with 2 moles RR1NH gave 90% NCC(S-):C(CN)SC(CN):C(CN)NRR1 (II) where R = R1 = Me (IIa) or Et or (NRR1 =) morpholino (IIb) or piperidino. II reacted with (MeO)2SO2 to give MeSC(CN):C(CN)SC(CN):C(CN)NRR1. Reaction of IIa or IIb with H2O2 gave the corresponding NCCH:C(CN)SC(CN):C(CN)NRR1, while only resinous products were obtained from the other II with H2O2.
 IT 28091-16-9P 28091-17-0P
 RI: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 28091-16-9 CAPLUS
 CN Fumaronitrile, [(1,2-dicyanovinyl)thio]morpholino-, (E)- (8CI) (CA INDEX NAME)

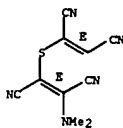
Double bond geometry as shown.



RN 28091-17-0 CAPLUS
 CN Fumaronitrile, [(1,2-dicyanovinyl)thio](dimethylamino)-, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



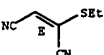
L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1963:70841 CAPLUS
 DOCUMENT NUMBER: 58:70841
 ORIGINAL REFERENCE NO.: 58:12100f-h
 TITLE: Preparation and study of the Faraday effect of several esters and the dinitrile of acetylenedicarboxylic acid as well as their addition compounds with thiols
 AUTHOR(S): Turpin, Andre; Voigt, Daniel
 CORPORATE SOURCE: Lab. Chim. Generale Minérale, Toulouse, Fr.
 SOURCE: Compt. Rend. (1963), 256, 1712-14
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB The following compds. were prepared: NCC.tpbond.CCN (I); RO2CC.tpbond.CCO2R with R = Me (II), Et (III), Pr (IV); NCC(SR):CHCN, with R = Et (V), Pr (VI), Bu (VII); and MeO2CC(SR):CHCO2Me, with R = Et (VIII), Pr (IX), and Bu (X). Their magneto-optical consts. were obtained and compared with those calculated by the method of Gallais, et al. (CA 55, 119701). The following rotations were obtained at $\lambda = 0.578 \mu$: (compound, observed Faraday rotation (microradians), calculated Faraday rotation (microradians)) I, 380, 340; II, 546, 497; III, 694, 643; IV, 838, 789; V, 915, 737; VI, 1000, 810; VII, 1099, 833; VIII, 1045, 893; IX, 1115, 966; X, 1190, 1039. The difference between the observed and calculated values is due to the effect of conjugation.
 IT 91466-95-6, Fumaronitrile, (ethylthio)- (?) 91467-44-6, Maleonitrile, (ethylthio)- (?) 91982-63-7, Fumaronitrile, (propylthio)- (?) 91982-64-8, Maleonitrile, (propylthio)- (?) 92203-33-3, Fumaronitrile, (butylthio)- (?) 92203-34-4, Maleonitrile, (butylthio)- (?) (magneto-optical rotation of)
 RN 91466-95-6 CAPLUS
 CN Fumaronitrile, (ethylthio)- (7CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 91467-44-6 CAPLUS
 CN Maleonitrile, (ethylthio)- (7CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 91982-63-7 CAPLUS
 CN Fumaronitrile, (propylthio)- (7CI) (CA INDEX NAME)

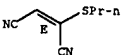
Double bond geometry as shown.

L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 91982-64-8 CAPLUS
 CN Maleonitrile, (propylthio)- (7CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 92203-33-3 CAPLUS
 CN Fumaronitrile, (butylthio)- (7CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 92203-34-4 CAPLUS
 CN Maleonitrile, (butylthio)- (7CI) (CA INDEX NAME)

Double bond geometry as shown.

